

1,4-Ethanonaphtho(1,8-ef)-1,4-diazepine, 2,3-dihydro-
59950-41-3 | DTXSID40208664

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 3.80e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.47e-01

Confidence level: 4.65e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Benzyl butyl phthalate</div> <div>Measured: 2.20e-04</div> <div>Predicted: 3.86e-06</div>	<div>Image not found</div> <div>Arsine, triphenyl-</div> <div>Measured: 3.92e-04</div> <div>Predicted: N/A</div>	<div>Image not found</div> <div>Isoamyl ether</div> <div>Measured: 6.80e-06</div> <div>Predicted: 1.87</div>
<div>Image not found</div> <div>1,2,3,4-Tetrachlorodibenzo-p-dioxin</div> <div>Measured: 2.00e-06</div> <div>Predicted: 1.73e-08</div>	<div>Image not found</div> <div>9,10-Dihydrophenanthrene</div> <div>Measured: 4.00e-05</div> <div>Predicted: 2.90e-04</div>	